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Obtaining Optimum Operation of CO_2 Absorption Plants

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Abstract

In this work a general optimization package is developed for CO2SIM. Three different methods of solving a specified case study have been tested. It gives a procedure which can be used for rapidly finding optimum operation conditions for a regeneration system in a CO_2 removal plant. The procedure is exemplified for a CO_2 absorption plant. The optimization procedure has been added as a new feature to the CO2SIM simulation software. To be able to examine the optimization module in a system perspective, campaign data from a pilot rig absorption/desorption unit has been used for initial comparison and validation. Thereafter the optimization tool was used to find out if the given case could be run in a more energy efficient manner.
It was found that finding optimums by "auto simulation of a matrix structure" was the most robust method.

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"Keywords: Optimization; CO2 capture; Simulation, MEA; Modeling"

1. Introduction

Since large scale CO_2 capture operations are very expensive to build for research purposes, process simulation and modelling have a profound role in evaluation of the various process alternatives. In this respect, system optimization is also required for energy cost cutting and energy efficiency improvement. Simulation and optimization studies are therefore essential for both design purposes as well as to find optimum operation conditions given a set number of process parameters. In order to find optimum operation conditions for a given absorption system, numerous simulations must be carried out.

This is the case because of the numerous process variables available for a CO_2 absorption plant. These simulations can carried out either manually by an operator or by optimization schemes in an automated fashion. As the size and complexity of the process flow sheets expands it becomes time consuming and difficult to find optimum

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operation conditions by manual simulations. It is therefore of great practical need to use optimization techniques to find a method to reduce these high numbers of manual simulations necessary to find process optimums.

Many commercial process simulators are capable of predicting the behaviour of the process in response to changes in the process structure or operating variables. However, there are no commercial simulators specifically designed for CO_2 post combustion absorption that includes routines for optimization. Furthermore, when general commercial simulators with optimization are used, their particular use for optimization is not a straightforward task as it demands for considerable manual and trial-and-error efforts by the user to adjust the variables to attain the objective function. Other issues are convergence issues appearing of the actual network.

2. Objectives

In this work different methods are tested in order to find optimum operation conditions for a given flowsheet. A systematic method for building optimization cases for any type of flowsheet configuration has been developed to automatically find optimum operation conditions. The procedure is exemplified for a CO_2 absorption plant. The optimization procedure has been added as a new feature to the CO2SIM simulation software. The CO2SIM model has been described in detail previously.[ii,iii,iv]

To be able to examine the optimization module in a system perspective, campaign data from a pilot rig absorption/desorption unit has been used for initial comparison and validation. Thereafter the optimization tool is used to find out if the given case can be run in a more energy efficient manner. Three different approaches have been used to find the most optimum variable settings to satisfy the objective functions that are not explicit mathematical equations but rather defined by the user based on a flowsheet network. Furthermore, constraints are given to the optimization problem, for example by specifying the CO_2 capture rate. It is believed that this procedure will significantly simplify evaluations and campaign designs of CO_2 absorption processes.

3. Specific system description

It is of great interest to find an operation with maximum net CO_2 removal at the lowest possible thermal energy requirement given a particular plant configuration. The procedure is therefore exemplified by using the method by finding the lowest specific reboiler duty given flue gas composition, as well as set process equipment sizes. In such a way, the system has a defined number of degrees of freedom. In the method a specified range will be supplied by the user for each degree of freedom. The optimization tool will thereby generate a simulation matrix with dimension equal to the degrees of freedom available (independent variables). The CO2SIM model will then be executed a number of times to find local optimums within the specified boundaries of the iteration variables. In this way the residual error function from the regression is minimized and optimum with respect to minimum specific reboiler duty will be found within the given user defined ranges.

4. The CO2SIM Optimization package

Description of CO2SIM Beta

The simulator is based on a flexible, modular, model building approach for allowing an evolutionary process simulator tool. The primary goal in this project is to provide a flexible and extensible simulation framework for solving a wide range of chemical processes related to CO_2 removal technologies. Due to the complex relationships among the units in a chemical plant, a hierarchical physical-functional decomposition of the process is defined. In this manner the simulation problem is broken down into modular components, and this operation is repeated until reaching an adequate level of representation.

The process simulator is based on a multi-layered architecture. The outer layer contains the topology of the process, i.e. the connected flow sheet. Each of the units (e.g. such as reactors, heat exchanger, etc.) belongs to the process unit layer. Finally, the specific properties of the system such as fluid properties, thermodynamics, etc., are contained in the process property layer.

Object-oriented architecture

All objects in the network structure are pointer handles, and are thus passed by reference and not by value. In this manner one will maintain data integrity and to keep all data updated throughout the network. A hierarchical and modular layout with class inheritance makes expansion of the model simple where each object down to the actual parameter level are defined as objects, encapsulating each parameter in the network at the lowest level. This structure is highly modular, making it possible to expand units and networks with new parameters and properties with no changes to the network code and only minimal changes to the Solver code accessing the new parameters.

5. Optimization framework in CO2SIM

Generating the optimization case

A code class was written in order to generate optimization problems for any type of network generated in CO2SIM. The class was written such that it could handle batch automatic experimental evaluation and comparative simulations from pilot plant data as well. The simulator then imports source experimental data via a common agreed translator nomenclature (this will be described in a following paper).

In regards to the optimization routines, the framework for inserting data into the flowsheet is used for definition of *n*-number of real variables within the allowed number of optimization parameters defining the network. An optimization algorithm will then maximize or minimize a user defined function (a cost function) defined from the general network.

The definitions are defined in the graphical user interface (GUI). For example, for a simple case, one parameter is marked as an optimization variable in the CO2SIM GUI as well as a user defined objective function (cost function). The objective function is designed as a function of the resulting data from one network simulation with possible constraints and is subjected to the optimization routines described later. A feasible solution that minimizes (or maximizes) the cost function subject to possible network constraints results in an optimal solution for the network. In Figure 1 is shown the process scheme for the optimization mode.

The code framework was principally designed to generate both single-variable optimization and multi-variable optimization cases in any type of process flowsheet, optimizing parameters or variables inside units or pipes.

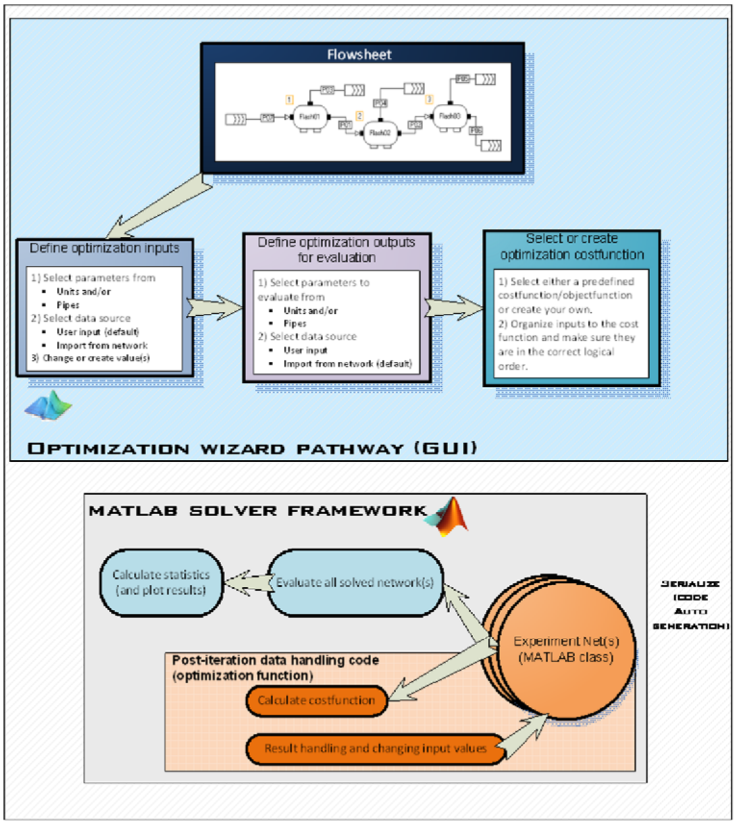

Figure 1. The conceptual process scheme for the optimization package in CO2SIM

Description of the optimization problem: Case Study: Aker Clean Carbon Mobile Test Unit (MTU)

The simulation task defined is to simulate the ACC Mobile Test Unit (MTU), owned and operated by Aker Clean Carbon, Norway. This is an integrated pilot plant with an absorber and desorber and connected unit operations. The particular case is a case study of a real flue gas input from the Longannet Power Station in Scottland. Details of the MTU and location in Scotland can be found elsewhere.[i]

The CO2SIM simulator was validated against results of the SINTEF pilot campaign for 30wt% monoethanolamine (MEA) solvent. The simulator was then used to find the lowest specific reboiler duty by varying amine circulation rate, concentration, reboiler duty and pressures in the regeneration section. Based on the validated pilot data, these process variable modifications could then be evaluated easily within a large operational regime in a short time.

A simplified schematic of the regeneration sections of the MTU (basic process configuration) is shown in Figure 2. Flow sheets are constructed from the CO2SIM GUI by "drag-and-drop" of the different unit operations and then connecting them altogether. The desorber-column used is a rate-based column model and further information can be found elsewhere.[ii,iii,iv,v] The column model in CO2SIM is highly non-linear due to large resulting source terms because of the fast chemical reactions taking place. Therefore, the flowsheet network was tested for convergence before optimization was started. The network solver developed uses direct substitution of each stream in the network in a sequential modular fashion with different modes of damping. For stability a method which has been proven sufficient for a large number of large flow sheets is to use adaptive continuation for the first couple network iterations.

6. Process configurations and definition

We have chosen to use a constant rich stream as the inlet to the optimization flowsheet. This inlet stream is based on loading the solvent to a point where it has an 85% degree to equilibrium, based on the inlet CO_2 partial pressure of the flue gas. This was found by using the absorber model as shown in Figure 2 and keeping the rich outlet from the absorber as input to the optimization network. For MEA it can be argued that it is possible to load the solvent significantly higher, however, it was decide that this was appropriate for relative comparisons of the regeneration section. Since we are interested in monitoring the regeneration of the solvent with an initial same loading level on the solvent, the absorber was not included in the optimization flowsheet. The absorber is therefore decoupled as shown in Figure 2. The Longannet Power Station flue gas content is shown in Table 1. The column specifications and solvent composition are shown in Table 2 and Table 3 respectively. A side stream is taken from the plant and tested on the MTU.

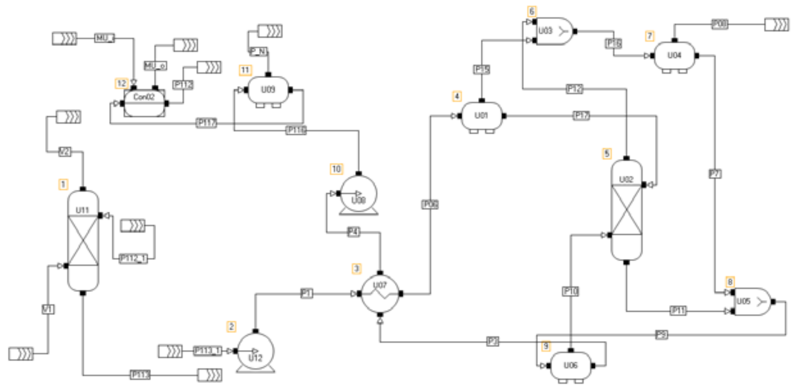

Figure 2: The conceptual process scheme for the optimization problem

Procedures for optimization

The CO2SIM software has a particularly powerful serialization functionality which makes auto generation of code possible directly to Matlab from the GUI. This means that any type of process flowsheet can be executed in Matlab and handled there. The GUI also, as mentioned earlier, sets up the optimization case based on the optimization outer shell.

Specific problem formulation

The three following criteria were necessary for defining the optimization problem:

1. *Generation of the objective function to be optimized*: The specific reboiler duty required for the given case was obtained from the post-iteration network data handling code to be minimized. Units are given as MJ/kg CO_2 removed.
2. *Network constraint function:* The CO_2 production rate is set to 51% removal from the rich solvent flow rate (for the MTU this means a constant removal rate of 103 kg/h).
3. *Definition of the optimization variables*: The essential process decision variables of the process are the *reboiler duty, solvent circulation rate, solvent concentration and reboiler pressure*.

Three methods of solution were tested for solving the problem: Solving the case directly using a constrained multivariable optimization algorithm, or converting the problem to an unconstrained multivariable optimization by solving the constraint function in an inner iteration loop, and lastly setting up a batch matrix structure of the different variables to find the global minimum manually in a post-simulation evaluation. The last option is time consuming and involves excessive simulations however, the procedure is robust within the given boundaries and the minimum can easily be visualized. This was used firstly to find the solution.

General data

Table 1: Sour Gas inlet

FLUE GAS DATA		
Name	***Value***	***Unit***
Flowrate	538	Sm^3/h
Flowrate 22.78	22.78	kmol/h
Gas Inlet Temperature	32.7	°C
Pressure	103	kPa a
CO_2	11.43	vol%
H2O	4.25	vol%
Inert	84.32	vol%

Finding optimums by auto simulation of a matrix structure: Method 1

The algorithm used for solution is the following:

Initialization:

1. Read flowsheet network
2. Define optimization variable Q reboiler and boundaries (Only one variable in this case and the optimization variables from the GUI is defined for the reboiler duty only).
3. Definition of objective function: Streams P113_1 and P08 are checked as evaluation streams defined from the GUI. Results of the function give the CO_2 Production rate (objective function, 51% CO_2 removal).
4. Set. solvent amine concentration in P113_1
5. Set. pressures in plant (reboiler, inlet flash and condenser)
6. Define the boundaries for the first iteration variable by creating a value range, for convenience the circulation rate is chosen with a value range from 65 to 120 kmol/h solvent.

Solve System:

1. Solve inner loop flowsheet with respect to CO_2 production rate, to yield the specific reboiler duty. (Produces the specific reboiler duty of the current network at the given circulation and removal rate.
2. Set new circulation rate and Solve inner loop
3. Once a range of circulation rates have been obtained, go to 5 and set new pressure.
4. Go to Solve system 1 and solve for new pressure.
5. Set new concentration and Solve system for new amine concentration.

Table 2: Column Data

ABSORBER:		
Name	*Value*	*Unit*
Geometrical data		
Height of packing	18.286	m
Diameter	0.397	m
Packing material	Mellapak 2X	
Specific surface of packing	205	m2/m3
Surface of packing	464.03	m2
DESORBER:		
Geometrical data		
Height of packing	7.81	m
Diameter	0.32	m
Packing material	Mellapak 2X	
Specific surface of packing	205	m2/m3
Surface of packing	126.28	m2

Table 3: Solvent data

NAME	***VALUE***	***UNIT***
Solvent	32% MEA	
Lean loading	0.15-0.28	
Abs. inlet temperature	18	°C
Abs. inlet Pressure	1.16	kPa g
Flow	95	kmol/h

Unconstrained optimization: Guarantee fulfilment of constrains by using internal zero point solver: Method 2

The same procedure is used here, except that an optimization algorithm is used instead of just running a grid of simulations and finding the minimum specific reboiler duty. MATLAB's fmincon was used here. A constraint function was defined even though a zero point inner solver ensured that the constraint was always fulfilled for each optimization iteration. The zero point solver developed is discussed below.

Constrained Multivariable Optimization: Method 3

Here no inner zero point solver was used where all optimization variables were handled by the optimization algorithm including the defined network constraint and objective function.

7. Results and discussion

In Figure 3 is shown the specific reboiler duty as function of solvent flow rate at different reboiler/stripper pressures. The amine concentration is constant at 30wt% MEA. An optimum operation with lowest specific reboiler duty at each pressure condition is shown. These results are plotted based on the procedure running auto simulation of a matrix structure described as Method 1. This is a robust method for plotting the different efficiencies and obtaining minimums. The internal loop zero finding procedure guarantees that the network iterates to the specified CO_2 removal rate based on the defined objective function from the GUI. A Newton-Raphson solution scheme was used with step size control and plotting features. It was found that this solution strategy performed better than the MATLAB solver "fsolve". The reason for this was that perturbations in the iteration variable x (reboiler duty) often give small responses in the functions to be minimized around the first iterations for obtaining the initial Jacobi. This appeared even though the problem was scaled by normalization towards the initial values. As a consequence the relative change in the iteration variable (x) was less than the relative tolerance set on x and the optimizer did not converge properly. Therefore a Newton-Raphson method was coded that included user defined incremental start point for iteration. The step size was controlled to keep flowsheet network robustness.

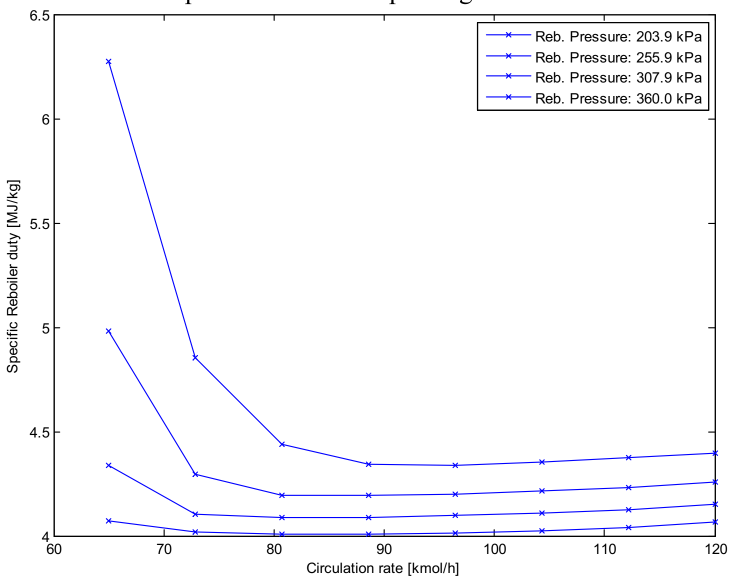

Figure 3: Specific reboiler duty as function of circulation rate 30wt%MEA

As already noted, the problem with this method is that it is time-consuming since numerous simulations are carried out far away from the optimum because there is no optimization algorithm being used. Also, the accuracy of the minimum depends on the static grid size that is manually chosen when defining the bounds.

Using Method 2 the minimum was found; however, using the same interval in circulation rate, it took about the same time as with Method 1. MATLAB's fmincon was used with the 'interior-point' algorithm option, which always honours the specified boundaries on the iteration variables.

When testing Method 3, the definition of the flowsheet constraints in the outer optimization algorithm as well as minimizing the objective function showed to be more problematic as the solution was very dependent on the initial guesses. This is due to the requirement that with the current problem setup was within the feasible solution rage with respect to the constraint, thus yielding solutions with constraint violations. The issue seemed to be that, usually, the initial problem would have a value slightly outside the feasible solution range.

To resolve the problem a penalty function was employed. The idea here is to transform the problem into a problem where a single unconstrained object function is minimized. Analogous to Method 2, however without the inner loop solver that removes the need for a constraint function. This includes a series of minimizations of the unconstrained function where the penalties are changed at every new iteration to force minimizing the constraint. Still, when using this technique, the initial guess had to be very close to the problem solution. The authors are therefore continuing working on solving this strategy by utilizing alternative algorithms.

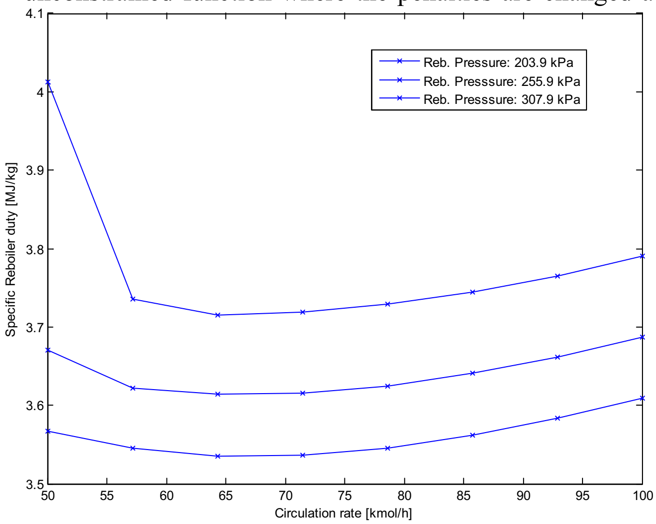

Figure 4: Specific reboiler duty as function of circulation rate 40wt%MEA

Evaluation of the simulation results

In Table 4 and Table 5 are shown the minimum values found for the standard pilot configuration using 30wt% MEA and 40wt% MEA respectively. The minimum specific reboiler shows a minimum at a given circulation rate, concentration and pressure. It is clear that an increased pressure in the reboiler will reduce the specific reboiler duty. The effect is due to the increase temperature in the reboiler which increases both the water and CO_2 partial pressures. The degree of this effect is given by the VLE model. At 256 kPa the reboiler temperature is raised to 129°C. It is evident that this has a positive effect on the steam consumption. A temperature above 129°C is too high for an MEA process, but it does indicate the potential that lies in increasing the reboiler temperature, or in other words, to develop a solvent that has better stability at high temperatures. An added bonus not shown here is the possible reduced recompression cost. The recompression cost can be somewhat reduced when going from 2 to 3 bar CO_2 outlet pressure.

Table 4: Summary minimums at different solvent concentration and reboiler pressure

MEA conc.	Reboiler Pressure	Reboiler temp.	Circulation rate	Specific reboiler duty
30wt%	203.9	122.1	96.42	4.33
	255.9	129.5	88.57	4.19
	308.0	136.0	80.71	4.09
40wt%	203.9	124.1	64.28	3.71
	255.9	130.6	62.18	3.61
	308.0	135.9	60.45	3.53

Although the heat duty figures given here are reasonable, they are not intended to be accurate as absolute optimized numbers. Ideally, by maximizing the loading obtainable from the absorber and at the same time avoiding the pinch region in the desorber during stripping, it is possible to lower steam usage substantially. In this example an 85% degree of approach to equilibrium is assumed in the absorber based on CO_2 loading. Also, the model flow sheet does not consider advanced flowsheet configurations which can potentially lower the specific reboiler duty substantially. The simulations with 40wt% MEA solution may not be accurate since the equilibrium model used in this work has not been validated for these high concentrations. For the purpose of studying desorber performance characteristics for an MEA plant with given operating conditions; the specific steam consumption parameter should therefore be regarded as a relative number only, since the purpose of the present paper is to study variations in this for testing the new optimization methods in CO2SIM. More precisely, the only validated results from pilot plant data (the SINTEF pilot rig) are the simulations at 30wt% at a reboiler pressure at 203 kPa.

8. Conclusions

In this work a general optimization package is developed for CO2SIM. Three different methods of solving have been tested. It gives a procedure which can be used for rapidly finding optimum operation conditions for a regeneration system in a CO2 removal plant. It was found that finding optimums by "auto simulation of a matrix structure" was the most robust method. More work will be completed in order to test alternative optimization algorithms.

For the optimization case study the basic configuration of the Aker Clean Carbon MTU basic unit configuration was simulated, based on the size of the columns, and optimized with respect to lowest specific reboiler duty at a given capture rate.

Table 5: Summary best performing case 85% to equilibrium at a reboiler pressure of 203.9

		30%wt MEA	40%wt MEA
Rich Flow	kmol/hr	96.42	64.28
	Kg	2263	2263
Rich Loading		0.449	0.449
Lean Loading		0.216	0.211
CO_2 stripped	kmol/hr	2.343	2.343
	kg/hr	103.1	103.1
Reb. Duty	kW	124	105
Specific Duty	MJ/kg	4.33	3.71

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Literature Cited

i Aker Clean Carbon homepage: http://www.akercleancarbon.com/

ii Tobiesen F.A., Juliussen O., Svendsen H.F., "Experimental Validation of a Rigorous Absorber Model for CO2 Postcombustion Capture", AIChE Journal (2007), 53(4),846-865

iii Tobiesen F.A., Juliussen O., Svendsen H.F., "Experimental Validation of a Rigorous Desorber Model for CO2 Postcombustion Capture", Chem. Eng. Sci (2008), 63,10, 2641-2656

iv Tobiesen A. and Svendsen H.F., Study of a Modified Amine Based Regeneration Unit, Ind. Eng. Chem. Res., 2006, 45, 2489-2496

v Tobiesen, F.A. and Dorao, C.A., A simulation study of alternative process configurations for a CO2 absorption plant using CO2SIM, in proceedings of the 9th International Conference on Greenhouse Gas Control Technologies - GHGT-9, November 16-20, 2008, Washington DC, USA.